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Low-dimensional structures generated by misfit dislocations in the bulk of $Si_{1-x}Ge_x$/Si heteroepitaxial systems

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The capability of misfit dislocations to generate nanostructures in the bulk of $Si_{1-x}Ge_x$/Si heteroepitaxial systems is demonstrated. It is shown that dislocation slip originating from compositionally graded $Si_{1-x}Ge_x$ layers can produce a range of low-dimensional structures including nanowires, nanodots, and mosaic superlattices. Formation of the nanostructures is achieved in parallel processing, through a simple two-step cycle which includes growth of layered planar structures and postgrowth annealing.
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Dislocations are attractive tools for the structuring of crystalline materials with atomic scale precision, since they operate over macroscopic distances and induce, at the same time, only very small relative displacements of atoms in a crystalline lattice.[1] Structuring of solids by the introduction of dislocations can be achieved in two principally different ways. The first and conventional one is to load a crystal with mechanical forces produced by external devices which implies the crystal with dislocations to be a *passive* element in the structuring process. Such an approach lies at the foundation of macroscopic forming operations and has recently been used for the formation of semiconductor nanostructures:[2] quantum wires have been formed by means of dislocation slip induced by a uniaxial external load in GaAs/GaInAs heteroepitaxial systems. In the present letter we elaborate on a novel, alternative approach in which highly metastable, compositionally graded $Si_{1-x}Ge_x$ layers serve as *active* elements in the structuring of crystalline material deposited on top of the graded films. Our recent studies showed that dislocation slip originating from the graded layers can be used for the fabrication of a variety of zero- and one-dimensional nanostructures on the *surface* of the epitaxial system.[3] In the following, we will demonstrate that the similar structuring principle can be used for the fabrication of nanostructures in the *bulk* of the epitaxial film (bulk nanostructures) which may be useful for the studies of physics of low-dimensional systems.

The approach is based on the property of dislocation-generation sources in SiGe/Si systems to form dislocation bunches (see e.g., Ref. 4). In the extreme situation, when the relaxation of the mismatch strain occurs far from equilibrium, the misfit dislocations generated in compositionally graded layers appear to be confined to very narrow slip bands.[5] This property leads to the basic concept of nanostructuring which includes two stages (Fig. 1):

(i) Growth of metastable (dislocation-free) heteroepitaxial system which consists of a compositionally graded $Si_{1-x}Ge_x$ buffer layer *(active element)* and a uniform $Si_{1-x}Ge_x$ layer *(passive element)* comprising a quantum well and a superlattice [Fig. 1(a)].

(ii) High-temperature annealing of the grown system which results in dislocation slip leading to the formation of nanostructures as shown in Fig. 1(b).

The samples for the present study were grown by molecular-beam epitaxy (MBE) on (001) Si substrates and include graded layers identical to those used in our previous work[3] for the formation of surface nanostructures. In the experimental system designed for the formation of bulk nanostructures, two types of layered structures are included in the uniform top layer:

(i) 5- and 7-nm-thick silicon quantum wells (QWs) and

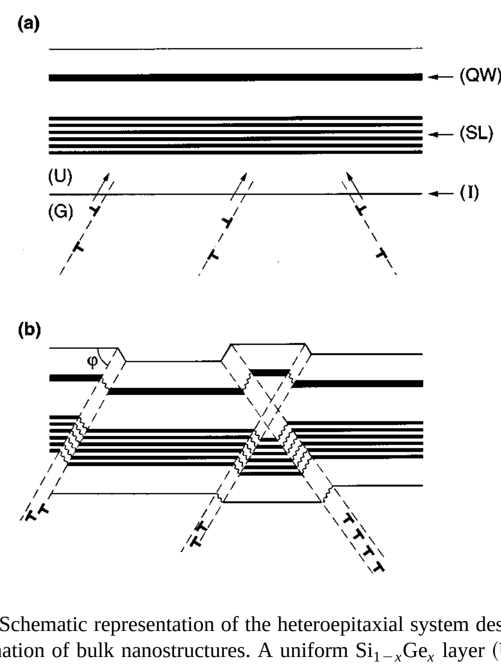

FIG. 1. Schematic representation of the heteroepitaxial system designed for the formation of bulk nanostructures. A uniform $Si_{1-x}Ge_x$ layer (U) grown on top of the compositionally graded layer (G), includes a quantum well (QW) and a superlattice (SL). (a) The initial structure and the generation of misfit dislocations. Multiplication sources activated in the graded layer during high temperature annealing produce dislocation loops ($\top\perp$). The upper segments of loops glide through the interface (I) into the top layer, displace its fragments and, finally, disappear emerging on the surface. (b) The final structure of the object. The dashed lines denote the slip regions.

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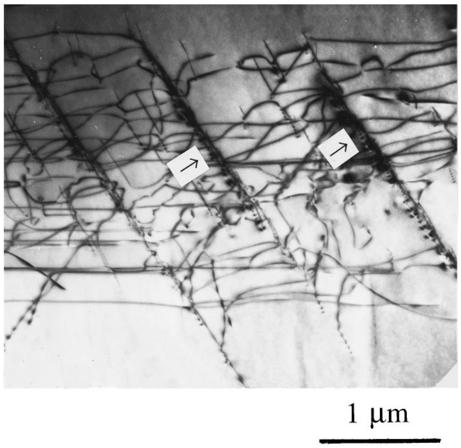

FIG. 2. Cross-sectional TEM image in [110] projection of the dislocation structure formed in the compositionally graded layers during annealing at 800 °C for 10 s. Two of the shear bands composed of 60° dislocations propagating perpendicular to the cross-sectional plane are denoted by the arrows.

(ii) a compositionally modulated structure (CMS) with a wave length of 4 nm.

The modulation of the alloy composition in the latter structure was achieved by using a combined effect of the deposition geometry and the substrate rotation:[6] Due to a nonuniformity of the Si and Ge atomic fluxes across the wafer the alloy composition in the growth direction is modulated with a wavelength $\lambda = R_T/\nu$, where R_T is the total (Si plus Ge) deposition rate and ν is the number of revolutions/s. After growth the samples were annealed either directly in the MBE chamber in ultrahigh vacuum (UHV) conditions or by rapid thermal annealing (RTA) at 800 °C for 10 s. The samples were characterized by cross-sectional transmission electron microscopy (TEM).

The cross-sectional TEM image shown in Fig. 2 illustrates the typical dislocation structure generated in the compositionally graded layers during RTA at 800 °C. Well-defined narrow shear bands composed of 60° misfit dislocations propagating in {111} slip planes perpendicular to the cross-sectional plane are seen in this figure. Figures 3(a) and 3(b) which are enlarged TEM images of the sample shown in Fig. 2, illustrate typical sets of low-dimensional structures generated by the dislocation slip. In Fig. 3(a), two regions of dislocation slip parallel to (111) and $(1\bar{1}1)$ slip planes are distinguished. The slip regions are very narrow, characterized by a width of about 6 nm, which is consistent with previous TEM findings[5] showing that the dislocations in the slip bands glide on parallel, closely spaced glide planes. The planarity of the layer elements composing the whole structure is broken in the slip regions by a superposition of displacement steps caused by individual dislocations. The important feature of this volume pattern is that near the intersection point of the (111) and $(1\bar{1}1)$ slip regions the width of the elements cut from quantum wells and the compositionally modulated structure becomes comparable to their thicknesses and, therefore, they become one-dimensional (1D) bulk structures (nanowires). The generation of 1D nanowires is further developed in Fig. 3(b). In this case two close-spaced parallel slip regions confine a *stair-set* of nanowires of equal width (~10 nm). This example clearly illustrates the great potentials of this new structuring technique in realizing many identical nanostructures distributed over a large volume.

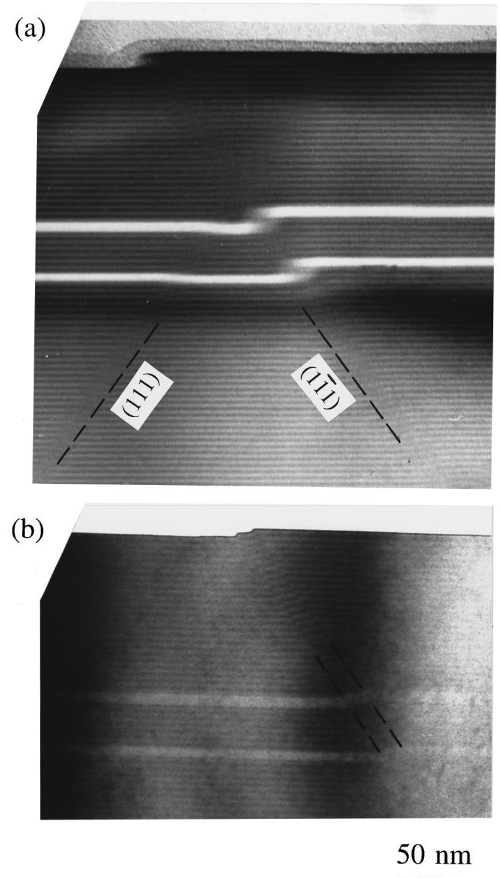

FIG. 3. [110] cross-sectional TEM images of typical low-dimensional, bulk structures observed after RTA in the top $Si_{0.8}Ge_{0.2}$ uniform layer comprising two Si quantum wells and the compositionally modulated structures. (a) The set of nanostructures generated by the dislocation slip in two intersecting bands (indicated). (b) Nanowires generated by two closely spaced parallel slip bands (indicated).

Zero-dimensional (0D) bulk structures cannot be seen in the cross-sectional TEM images. However, 0D surface structures have been revealed in atomic force microscopy (AFM) images of the surface of this sample, at the intersection of perpendicular pairs of narrow shear bands. This implies that similar perpendicular displacements in the bulk form 0D bulk structures. It should be emphasized that, due to the simple geometrical relationship [see Fig. 1(b)] between the surface and bulk morphologies, the lateral position of any particular bulk nanostructure can easily be identified by the position of its surface ''satellite.'' This feature can be very helpful for studies of physical and functional properties of the nanostructures by a number of nanoprobe techniques, e.g., by near-field scanning optical microscopy or ballistic electron emission microscopy.

The plastic displacements caused by misfit dislocations in heteroepitaxial semiconductor systems have always been considered harmful to electronic devices. In this respect the work presented here is the first real attempt to take advantage of these displacements, which are shown to be capable of producing quantum wires and dots. The bulk nanostructures found in this study are interesting, not only as individual elements: Considering the patterned structure as a whole system we recognize that the structuring by the slip bands provides formation of a new type of *disordered superlattices*, where superlattice elements are displaced with respect to each other in the growth direction, or even a *mosaic superlattice*, if the local tilts and rotations induced by the dislocation bands[7] are taken into account. The interest in disordered superlattices[8] is caused by the fact that luminescence from such systems can be enhanced as compared to that from ordered structures. Obviously, further studies are needed to evaluate the ability of the dislocation-induced steps to confine charge carriers.

There are different options in the preparation of our systems which provide control of the dislocation morphologies in the graded layers and, thus, of the displacements patterns. Independent means for controlling the vertical displacements and the lateral length scale of the displacement patterns were discussed in our previous article.[3] Another possible way of changing the geometry of the slip band patterns is to use Si substrates with different deliberate miscuts; it was shown in Ref. 7 that even a relatively small miscut ($\sim 2°$) of the Si substrate from the exact (001) orientation can significantly enhance the generation of misfit dislocations in one slip system while suppressing it in another slip system.

Looking at the system depicted in Fig. 1 from a general point of view one recognizes that this system possesses the structure and functionality of a machine.[9] Similar to other mechanical devices it possesses the *generator* (the compositionally graded layer which generates the mechanical displacements), *energy supply* (elastic energy stored in the system during growth), and the *interface* (the atomic interface between the graded and the top layer which provides ''transmission'' of the crystallographic slip induced in the generator). Like any other machines this system belongs to the category of open dissipative systems which do their work through energy and entropy exchange[5] with the external world. In this respect our systems are the first realization of *dislocation machines* — mechanical devices in which dislocations serve as key components.

In conclusion, new capabilities of misfit dislocations for spatial structuring of $Si_{1-x}Ge_x/Si$ epitaxial systems at the nanometer length scale have been elucidated. We find that the crystallographic slip originated in the metastable, compositionally graded $Si_{1-x}Ge_x$ layers can be used for the reduction of the dimensionality of quantum wells and superlattices, resulting in the formation of a range of one- and zero-dimensional, bulk nanostructures. A strong resemblance to conventional machines has lead to the term *dislocation machines* for these systems.

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[9] A dictionary definition of a machine is ''any system, usually of rigid bodies, formed and connected to alter, transmit, and direct applied forces in a predetermined manner to accomplish a specific objective, such as the performance of useful work'' [K. E. Drexler, *Engines of Creation* (Anchor, New York, 1986)].